On Computer Algebra Generation of Symplectic Integrator Methods

or

Of Headaches, Nightmares, and Algebra

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Note: the full set of slides for this talk is located on the web at

http://aa.usno.navy.mil/murison/talks/

ON COMPUTER ALGEBRA GENERATION OF SYMPLECTIC INTEGRATOR METHODS

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Abstract

Most symplectic integrators used in solar-system dynamics are second-order in the time step τ. Typically, the Hamiltonian is divided into a Keplerian piece H_A and a smaller perturbative component H_B. We can take advantage of the disparity in relative magnitude of these components to define a second small parameter, call it $\varepsilon = \frac{|H_B|}{|H_A|} \ll 1$, and use this to obtain a "partially" higher-order method.

Adopting a Lie series approach, one can, for a given order-N method, examine the τ^{N+1}, τ^{N+2}, etc. error terms. Each of the $2^k - 2$ subterms of the coefficient of the τ^k error term has an associated factor of ε raised to a power ranging from linear to $k-1$. By including adjustable parameters in each evolution operator $exp(\tau\{\cdot,H_A\})$ or $exp(\tau\{\cdot,H_B\})$ in the trial method (composed of a combination of these operators) that approximates the true Hamiltonian evolution operator $exp(\tau\{\cdot,H_A + H_B\})$, one can in principle eliminate specified subterms in specified error terms. For example, a second-order method chosen to eliminate the τ^3 subterms linear in ε can, depending on the magnitude of ε, produce a quasi-third-order method. In practice this process boils down to generating then solving systems of nonlinear polynomial equations particular to the trial method.

A computer algebra program has been developed that automates the generation and solution of the equations that result from requesting a specified method of order N. This task is tedious due to the noncommutative algebra involved in the series expansions and subsequent algebraic manipulations, but computers are well-suited for handling such tedium. Once a method, or set of equivalent methods, has been found, the program then generates and solves a second set of equations for parameter solutions whereby subterms of specified powers in ε are eliminated for successive τ^{N+1}, τ^{N+2}, etc. terms in the overall error expression.

The project has, in these initial stages, been at least partially successful. Experiences and results to date will be presented.

Symplectic Integrator Micro-Tutorial

- Hamilton's equations

$$\frac{d\vec{q}}{dt} = \frac{\partial H}{\partial \vec{p}}, \qquad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{q}}$$

- Poisson bracket

$$\{F, H\} \equiv \frac{\partial F}{\partial \vec{q}} \cdot \frac{\partial H}{\partial \vec{p}} - \frac{\partial F}{\partial \vec{p}} \cdot \frac{\partial H}{\partial \vec{q}} \qquad \longrightarrow \qquad \frac{d\,\cdot}{dt} = \{\cdot, H\}$$

- Equations of motion

$$\frac{d\vec{\xi}}{dt} = \{\vec{\xi}, H\} \qquad \vec{\xi} \equiv (\vec{q}, \vec{p})$$

- Formal Solution

$$\begin{aligned} \vec{\xi}(t) &= e^{\tau\{\cdot, H\}}\vec{\xi}(t-\tau) \\ &= \left(1 + \tau\{\cdot, H\} + \tfrac{\tau^2}{2}\{\cdot, H\}^2 + \ldots\right)\vec{\xi}(t-\tau) \end{aligned}$$

$$\tau \equiv t - t_0 \qquad \{\cdot, H\}^2 = \{\{\cdot, H\}, H\}$$

- Recast as a mapping or evolution operator:

$$S(\tau) \equiv e^{\tau\{\cdot, H\}}$$

$$\vec{\xi}(t) = S(\tau)\vec{\xi}(t-\tau)$$

The mapping "updates" the system to the next time step — the basis for a symplectic integration algorithm

Symplectic Integrator Micro-Tutorial (cont.)

- Split the Hamiltonian into two parts

$$H = H_A + H_B$$

also define operators $A \equiv \{\cdot, H_A\}$ $B \equiv \{\cdot, H_B\}$

  - e.g., a Keplerian part and a perturbative part
  - Then we can write

$$\begin{aligned} S(\tau) &= e^{\tau(A+B)} \\ &= 1 + \tau(A+B) \\ &\quad + \tfrac{1}{2}\tau^2(A^2 + AB + BA + B^2) + \ldots \end{aligned}$$

- Multiplication is noncommutative: $[A, B] \equiv AB - BA \neq 0$
  - Makes algebra more difficult
- Practical algorithm: take separate "A" and "B" steps

$$\begin{aligned} S_A(\tau)S_B(\tau) &= e^{\tau A}e^{\tau B} \\ &= 1 + \tau(A+B) \\ &\quad + \tfrac{1}{2}\tau^2(A^2 + 2AB + B^2) + \ldots \end{aligned}$$

$$S_A(\tau) \equiv e^{\tau A} \qquad S_B(\tau) \equiv e^{\tau B}$$

- Differs from the real Hamiltonian operator starting in the second-order term
  - Hence, two exponential operators gives us a first-order symplectic method

Symplectic Integrator Micro-Tutorial (cont.)

- Here's the trick: assemble a sequence of exponential operators $S_A(\alpha_k\tau)$, $S_B(\alpha_k\tau)$ and judiciously choose coefficients α_k to match the true evolution operator to a given order in the time step.
- Example: three exponentials yield second-order methods
  - The approximate Hamiltonian operator

$$
\begin{aligned}
\tilde{S}(\tau) &\equiv S_A(a\tau)S_B(b\tau)S_A(c\tau) \\
&= e^{a\tau A}e^{b\tau B}e^{c\tau A} \\
&= (1 + aA\tau + \tfrac{1}{2}a^2A^2\tau^2 + \ldots) \\
&\quad \cdot(1 + bB\tau + \tfrac{1}{2}b^2B^2\tau^2 + \ldots) \\
&\quad \cdot(1 + cA\tau + \tfrac{1}{2}c^2A^2\tau^2 + \ldots) \\
&= 1 + [bB + (a+c)A]\tau \\
&\quad + [\tfrac{1}{2}(a+c)^2A^2 + abAB \\
&\qquad + bcBA + \tfrac{1}{2}b^2B^2]\tau^2 \\
&\quad + \ldots
\end{aligned}
$$

  - Difference from the true Hamiltonian operator

$$
\begin{aligned}
\tilde{S}(\tau) - S(\tau) = &\ [(a-1+c)A + (b-1)B]\tau \\
&+ [\tfrac{1}{2}(a+1+c)(a-1+c)A^2 \\
&\quad + (ab - \tfrac{1}{2})AB + (bc - \tfrac{1}{2})BA \\
&\quad + \tfrac{1}{2}(b-1)(b+1)B^2]\tau^2 \\
&+ \ldots
\end{aligned}
$$

Symplectic Integrator Micro-Tutorial (cont.)

- Yields an overdetermined system of equations

$$
\begin{aligned}
b-1&=0\\
a-1+c&=0\\
(b-1)(b+1)&=0\\
2bc-1&=0\\
2ab-1&=0\\
(a+1+c)(a-1+c)&=0
\end{aligned}
$$

- Solution: $\{a=c=\frac{1}{2},\ b=1\}$
- The resulting method is second-order in the time step:

$$
\begin{aligned}
\tilde{S}(\tau) \;=\;& e^{\tau(A+B)}\\
&+\tau^3\left(\tfrac{1}{12}[B,B,A]-\tfrac{1}{24}[A,A,B]\right)\\
&+O(\tau^4)
\end{aligned}
$$

where

$$[A,A,B]\equiv[A,[A,B]]=A^2B-2ABA+BA^2$$

$$[B,B,A]\equiv[B,[B,A]]=B^2A-2BAB+AB^2$$

- This is the traditional symmetric second-order solution

Symplectic Integrator Micro-Tutorial (cont.)

- Using this approach, we can in principle construct approximate symplectic evolution mappings that match the "real" mapping to any given order in the time step
- Unfortunately, in practice this rapidly becomes very difficult
  - Number of equations to solve = $2^n - 2$
  - Complexity of individual equations grows rapidly with time step order n
  - polynomial order of equations goes as n

Two Useful Insights

1. We can adjust the parameters to optimize the error terms more to our liking
   - Make use of a second small parameter:

     $$H = H_A + \varepsilon H_B \qquad \varepsilon \ll 1$$

   - Add extra exponential operators
     - more parameters to play with
   - Selectively eliminate certain subterms in the time step error terms
   - For example, the traditional second-order evolution operator becomes

$$\begin{aligned}\tilde{S}(\tau) \; = \; & e^{\tau(A+B)} \\ & +\tau^3\left(\tfrac{1}{12}\varepsilon^2[B,B,A] - \tfrac{1}{24}\varepsilon[A,A,B]\right) \\ & +O(\varepsilon\tau^4)\end{aligned}$$

Remove this term and we have a quasi-fourth-order method

Two Useful Insights (continued)

2. Tedious and voluminous algebra: this is what computers are for!
   - General-purpose computer algebra systems (CAS)
     - Maple, Macsyma, Mathematica, Axiom, etc.
   - Symbolic programming languages enable
     - flexibility
     - algebraic sophistication
     - automation

Plan of Attack: a Two-Stage Process

1. Create a symplectic method, but include one or more additional exponential operators
   - Hard!
   - For example, a second-order method composed of more than three substeps
2. Solve for values of the extra parameter(s) that will eliminate the desired error subterms
   - Even harder!
   - Requires solving a second, usually nastier, set of polynomial equations
   - For example, in a second-order method, eliminate the subterms of the τ^3 error expression that are linear in the Hamiltonian operator *B*
     - If *B* is the small one, then the remaining dominant error terms go as $\varepsilon^2\tau^3$
     - This leaves us with an essentially fourth-order method(!)
   - Costs us extra exponential terms
   - There are cases where the extra cost is still significantly smaller than that of going to the full higher-order method

Symbolic Program SYMPLECTIC

- Implemented the Plan of Attack in the Maple symbolic algebra programming language
  - About 2500 lines of symbolic manipulation code
- Main parts:
  - symplectic method solver
    - specify
      - number of exponential operators
      - parameter list
      - time step order of method, n
      - number of time step error terms to calculate beyond n, so that we can play with them in the...
  - targeted subexpression eliminator
    - input
      - symplectic method (solution generated by first part)
      - method error expression (can be HUGE)
      - number of time step error terms beyond n in which to eliminate subterms that are linear in A (or B)
    - output
      - optimized solutions
      - the full corresponding solution errors

Symbolic Program SYMPLECTIC (continued)

- Subsystems:
  - polynomial equation set solver(!)
    - use the Maple general solver as kernel of algorithm attuned to our specific equation set form
    - in practice, employ *both* methods and eliminate duplicate solutions
  - noncommutative algebra procedures
    - series expansions
    - truncated series multiplication
    - transformations
    - factoring
  - plotting procedures
  - utility procedures
    - algebraic manipulators and expression simplifiers

Example of a [7,3] solution

notice the two free parameters

$$
\begin{aligned}
S_4 = \Bigg[\, a = -\frac{1}{3}\Bigg(\Bigg(\Bigg(&\frac{1}{6}\,\frac{(72c^3d^2 - 60c^2d^2 + 72c^3d^4 + 12dc^2 - 144c^3d^3 + 6cd + 72c^2d^3 - 6cd^2 - 1)\,Z1}{12c^2d^2 + 1 - 12dc^2} + \frac{1}{2}\big(\\
&-576c^3d^4 + 1 + 72c^2d^4 + 288c^3d^5 - 144c^4d^2 - 72c^2d^2 - 2592c^5d^5 - 864c^4d^6 - 864c^5d^3 \\
&+ 2592c^5d^4 + 1728c^4d^5 + 864c^5d^6 - 10cd + 192c^3d^2 + 18cd^2 - 1296c^4d^4 + 576d^3c^4 \\
&+ 24c^2d^3\big) \Big/ (12c^2d^2 + 1 - 12dc^2)\Bigg)(36c^2d^2 + 3 - 36dc^2)\Bigg) \Bigg/ \Bigg(\\
&(12c^2d^2 + 1 - 12dc^2)(-36dc^2 + 3 - 72c^2d^3 - 12cd + 108c^2d^2 + Z1) \\
&\left(\frac{1}{6}\,\frac{Z1}{12c^2d^2 + 1 - 12dc^2} - \frac{1}{2}\,\frac{-12c^2d^2 + 1 - 12dc^2 + 24c^2d^3 + 4cd}{12c^2d^2 + 1 - 12dc^2}\right)\Bigg)\Bigg), \\
b = -\frac{1}{6}\,&\frac{Z1}{12c^2d^2 + 1 - 12dc^2} + \frac{1}{2}\,\frac{12c^2d^2 + 1 - 12dc^2 + 4cd - 2d}{12c^2d^2 + 1 - 12dc^2},\ c = c,\ d = d,\ e = \frac{1}{3}\Bigg(\\
&\left(2\,\frac{cd(2c-1)\,Z1}{12c^2d^2 + 1 - 12dc^2} - \frac{(2c-1)(72c^3d^4 - 72c^3d^3 + 12c^2d^2 + 12dc^2 - 6cd^2 - 1)}{12c^2d^2 + 1 - 12dc^2}\right) \\
&(36c^2d^2 + 3 - 36dc^2)\Bigg) \Bigg/ \Bigg((12c^2d^2 + 1 - 12dc^2) \\
&(-36dc^2 + 3 - 72c^2d^3 - 12cd + 108c^2d^2 + Z1) \\
&\left(\frac{1}{6}\,\frac{Z1}{12c^2d^2 + 1 - 12dc^2} - \frac{1}{2}\,\frac{-12c^2d^2 + 1 - 12dc^2 + 24c^2d^3 + 4cd}{12c^2d^2 + 1 - 12dc^2}\right)\Bigg), \\
f = \frac{1}{6}\,&\frac{Z1}{12c^2d^2 + 1 - 12dc^2} - \frac{1}{2}\,\frac{12dc^2 - 1 + 24c^2d^3 + 4cd - 36c^2d^2}{12c^2d^2 + 1 - 12dc^2},\ g = -\frac{1}{3}\Bigg(\Bigg(\Bigg(\\
&\frac{1}{2}\,\frac{(2cd - 1)\,Z1}{12c^2d^2 + 1 - 12dc^2} \\
&- \frac{1}{2}\,\frac{-12cd^2 + 72c^3d^3 - 6cd - 72c^3d^2 + 108c^2d^2 + 1 - 12dc^2 - 72c^2d^3}{12c^2d^2 + 1 - 12dc^2}\Bigg) \\
&(36c^2d^2 + 3 - 36dc^2)\Bigg) \Big/ (-36dc^2 + 3 - 72c^2d^3 - 12cd + 108c^2d^2 + Z1)\Bigg)\,\Bigg]
\end{aligned}
$$

where

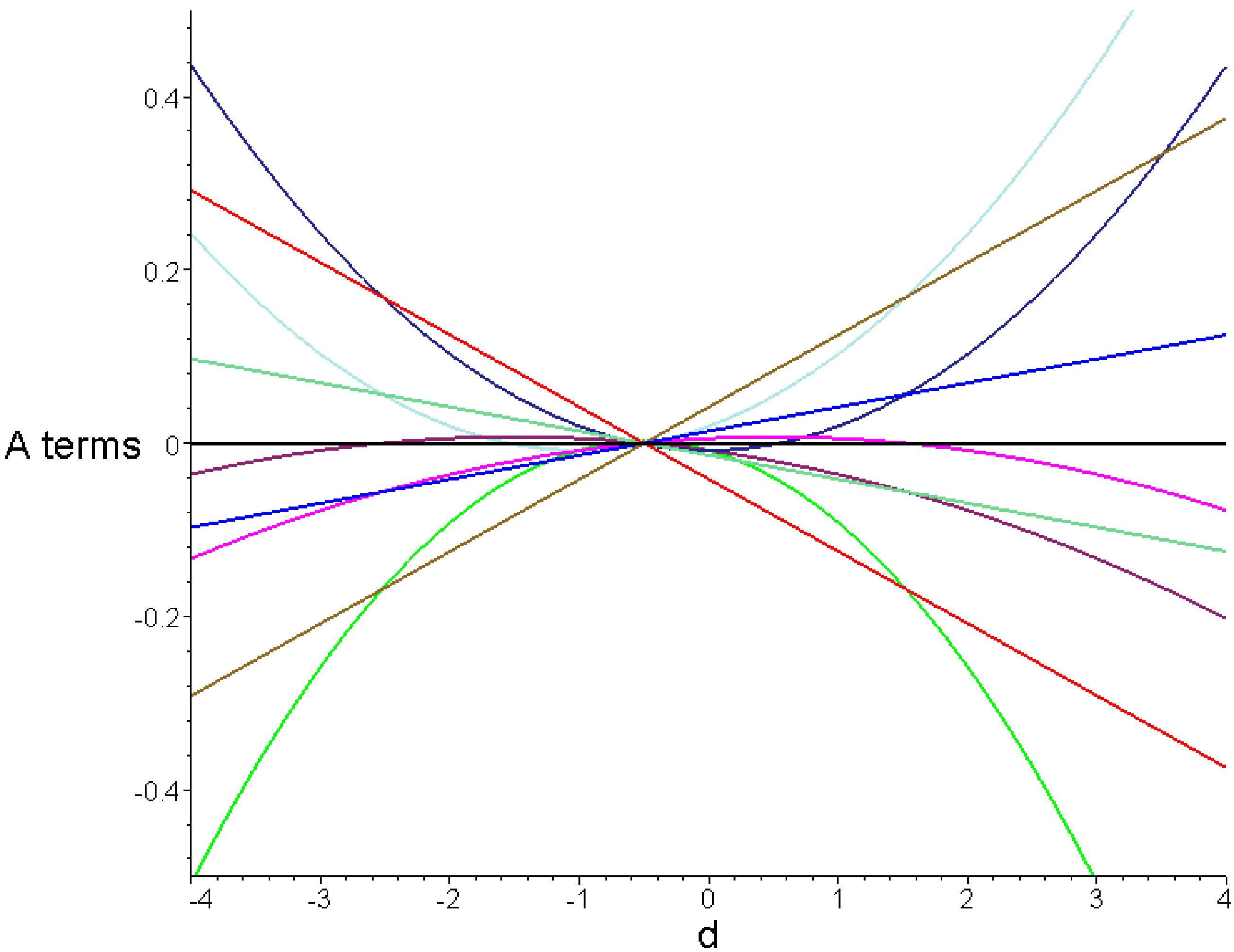
$$
\begin{aligned}
[\,\mathrm{sqrt}(&864c^3d^3 - 72dc^2 - 3 - 432c^2d^4 + 1296c^4d^2 + 216c^2d^2 + 72cd - 864c^3d^2 - 144cd^2 \\
&+ 1296c^4d^4 - 2592d^3c^4 + 432c^2d^3) = Z1\,]
\end{aligned}
$$

$C(\varepsilon_4) = 67532$ *multiplications* $+\ 14939$ *additions* $+\ 1372$ *divisions* $+\ 1298$ *functions*

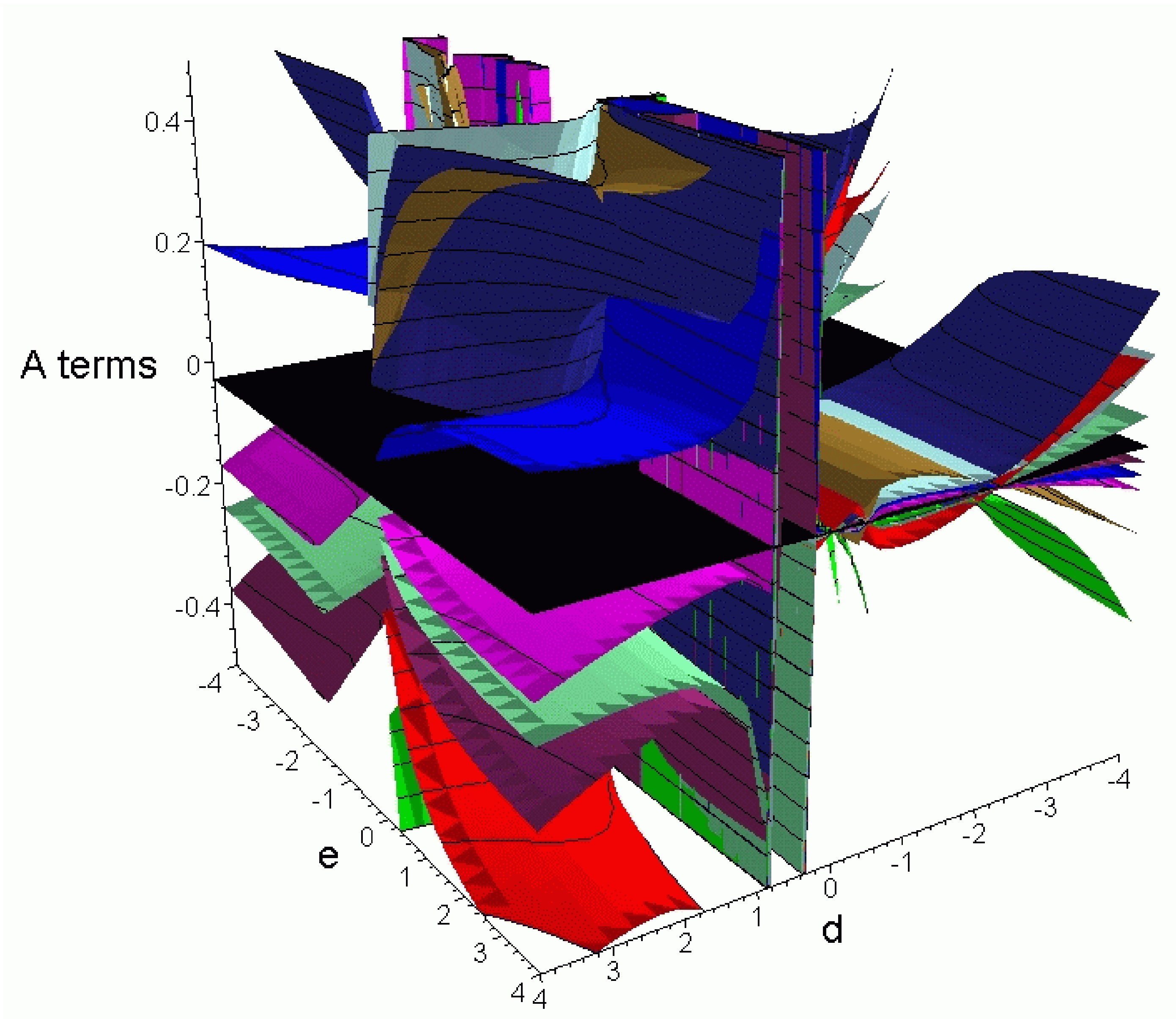
$C(\varepsilon_4) = 4849$ *additions* $+\ 45$ *divisions* $+\ 145$ *functions* $+\ 50360$ *multiplications*

size of error term

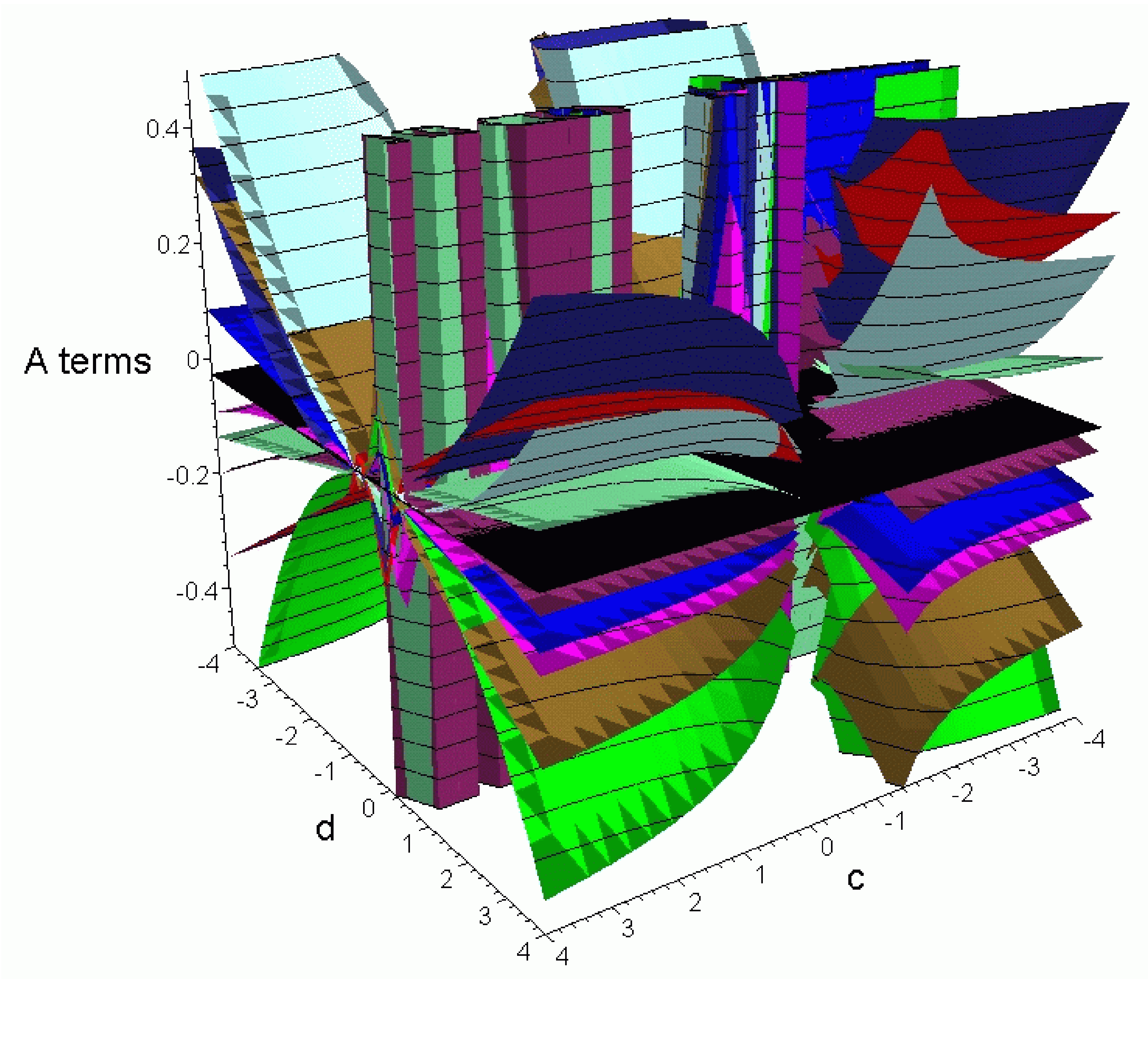
An example of linear-A terms to eliminate



An example of linear-A terms to eliminate



An example of linear-A terms to eliminate



Example of a [7,3] optimized solution

$$S_1 = \left[a = \frac{5}{24}, b = \frac{1}{2}, c = \frac{2}{3}, d = \frac{-1}{2}, e = \frac{-1}{24}, f = 1, g = \frac{1}{6} \right]$$

asymmetric solution

$$\begin{aligned}
\varepsilon_1 = \Big(& -\frac{1}{3456}\,\&^*(A,A,A,B) + \frac{1}{1152}\,\&^*(A,A,B,A) - \frac{1}{288}\,\&^*(A,A,B,B) - \frac{1}{1152}\,\&^*(A,B,A,A) \\
& + \frac{1}{144}\,\&^*(A,B,A,B) + \frac{1}{3456}\,\&^*(B,A,A,A) - \frac{1}{144}\,\&^*(B,A,B,A) + \frac{1}{288}\,\&^*(B,B,A,A) \Big)\tau^4 + \Big(\\
& - \frac{37}{23040}\,\&^*(A,A,B,A,A) + \frac{97}{34560}\,\&^*(A,A,B,A,B) + \frac{47}{34560}\,\&^*(A,A,A,B,A) \\
& - \frac{293}{207360}\,\&^*(A,A,A,B,B) - \frac{19}{46080}\,\&^*(A,A,A,A,B) - \frac{47}{23040}\,\&^*(A,A,B,B,A) \\
& - \frac{1}{320}\,\&^*(A,A,B,B,B) + \frac{1}{1080}\,\&^*(B,A,A,B,A) - \frac{1}{720}\,\&^*(B,A,A,B,B) - \frac{17}{138240}\,\&^*(B,A,A,A,A) \\
& - \frac{17}{51840}\,\&^*(B,A,A,A,B) + \frac{1}{480}\,\&^*(A,B,B,B,A) + \frac{1}{2880}\,\&^*(A,B,B,B,B) + \frac{11}{7680}\,\&^*(A,B,B,A,A) \\
& - \frac{1}{320}\,\&^*(A,B,B,A,B) + \frac{7}{5760}\,\&^*(A,B,A,B,A) + \frac{7}{960}\,\&^*(A,B,A,B,B) + \frac{1}{1280}\,\&^*(A,B,A,A,A) \\
& + \frac{1}{17280}\,\&^*(A,B,A,A,B) + \frac{1}{2880}\,\&^*(B,B,B,B,A) + \frac{1}{2880}\,\&^*(B,B,B,A,A) - \frac{1}{720}\,\&^*(B,B,B,A,B) \\
& + \frac{487}{207360}\,\&^*(B,B,A,A,A) + \frac{1}{480}\,\&^*(B,B,A,A,B) + \frac{1}{2880}\,\&^*(B,B,A,B,A) + \frac{1}{480}\,\&^*(B,B,A,B,B) \\
& - \frac{1}{320}\,\&^*(B,A,B,B,A) - \frac{1}{720}\,\&^*(B,A,B,B,B) - \frac{173}{34560}\,\&^*(B,A,B,A,A) - \frac{1}{720}\,\&^*(B,A,B,A,B) \Big)\tau^5
\end{aligned}$$

linear-A subterms are eliminated from the τ^4 term

Work Progress Report

- SYMPLECTIC is up and running, producing useful results
- Accessible [N,n] parameter space being explored
  - N = number of exponential terms $S_{A,B}(\alpha_k\tau)$
  - n = time step order of method, $O(\tau^n)$
  - symbolic algebra progress thus far:

n\N	2	3	4	5	6	7	8	9
1	-	-	-	-	-	-	-	-
2	×	✓	✓	✓	✓	✓		
3	×	×	×	×	✓	(✓)		
4	×	×	×	×	×	✓	(✓)	
5	×	×	×	×	×	×	×	×

    - Red shaded region is probably beyond current hardware and CAS capabilities
    - Each [N,n] case can yield *many* different solutions

- Optimized methods being compared with numerical solar system tests
- First AJ paper (of two) has been submitted

Preliminary Numerical Results

- Ran two 10,000-year cases:

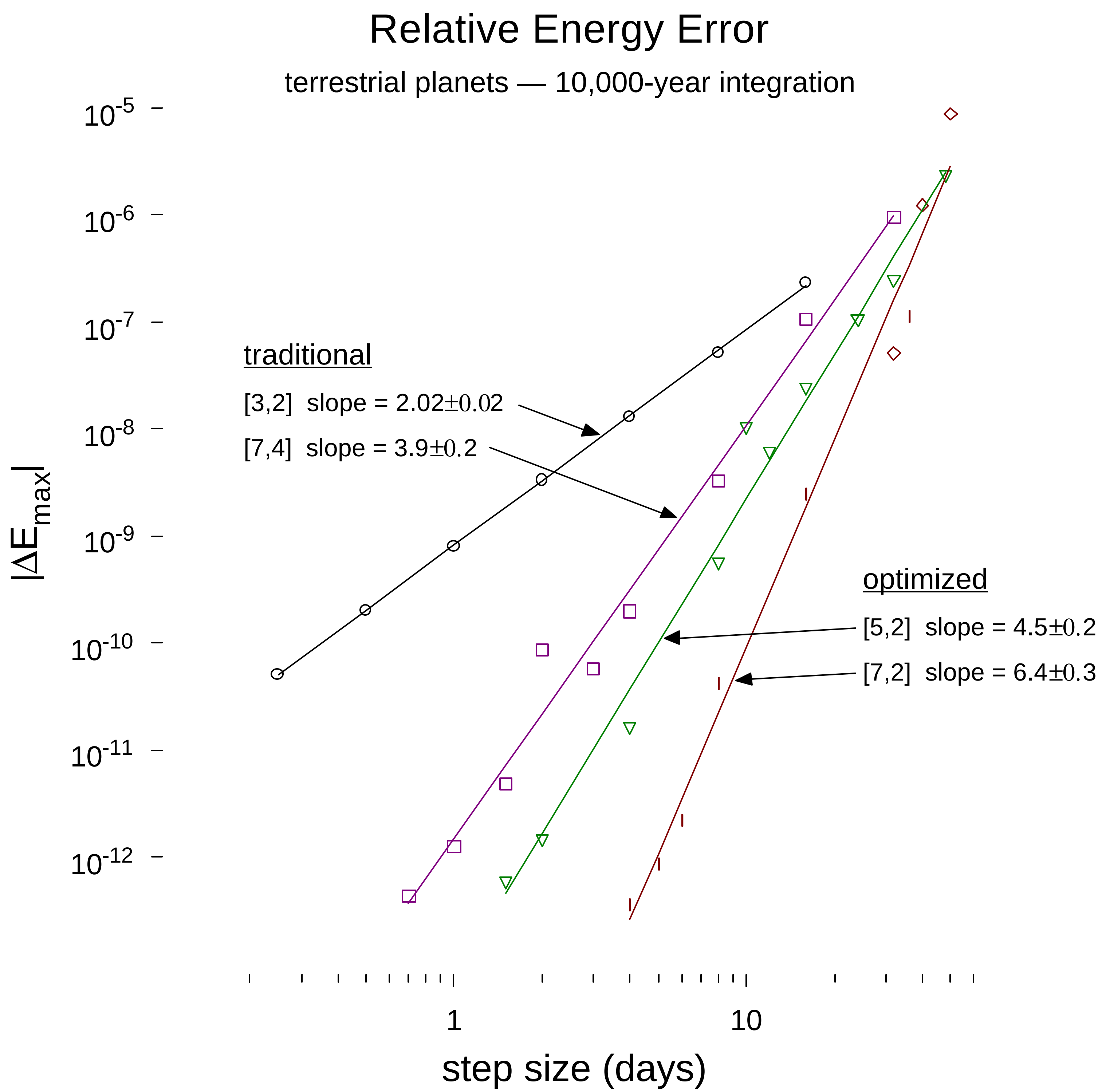
    1. terrestrial planets only ($\varepsilon \sim 10^{-5}$)
    2. all 9 planets ($\varepsilon \sim 10^{-3}$)

- three diagnostic parameters:
    - step size h
    - max energy error
    - elapsed CPU time

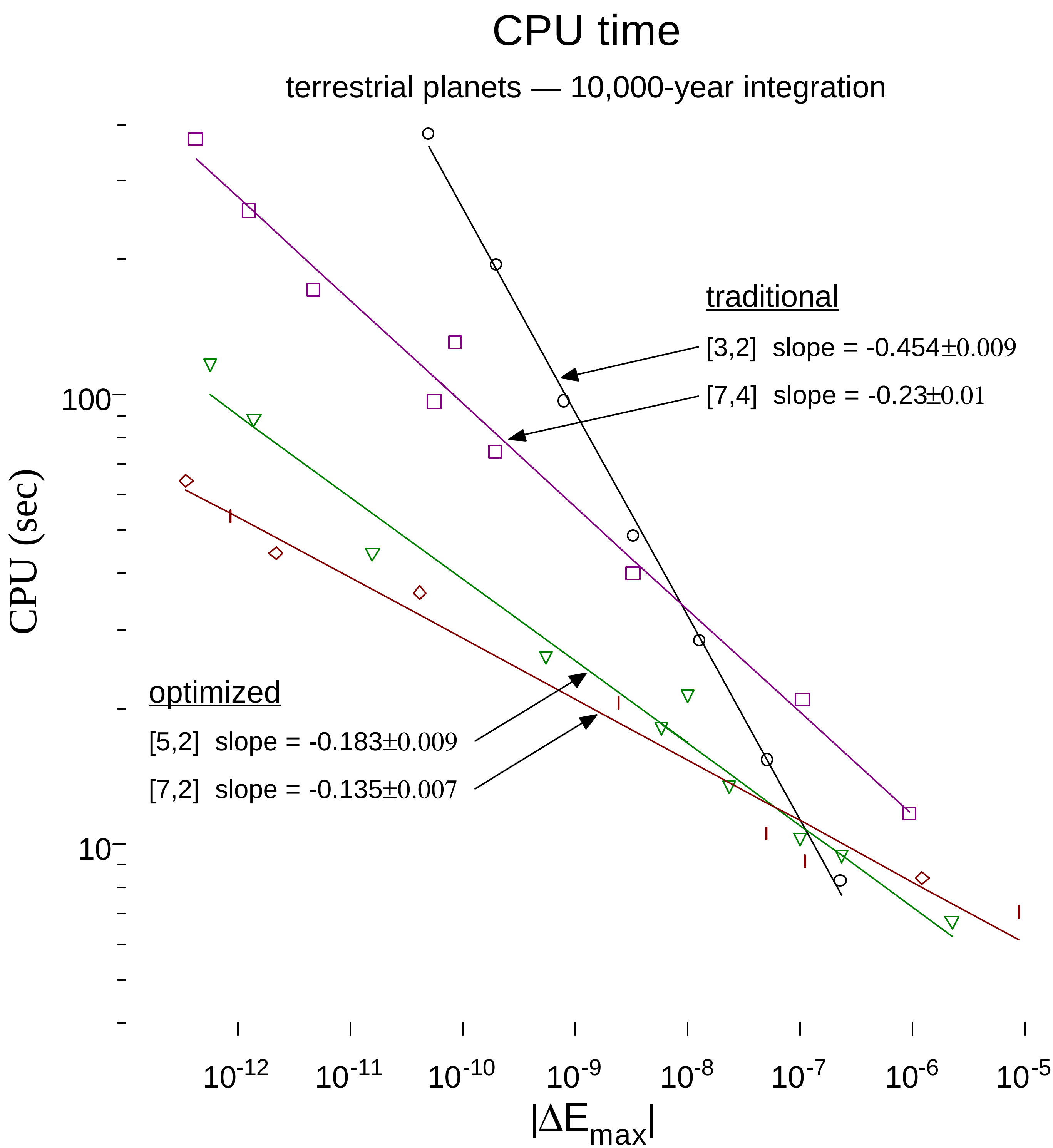
- Compared two selected methods (of many), from among the optimized [5,2] and [7,2] solutions, with the traditional 2nd and 4th order methods [3,2] and [7,4]

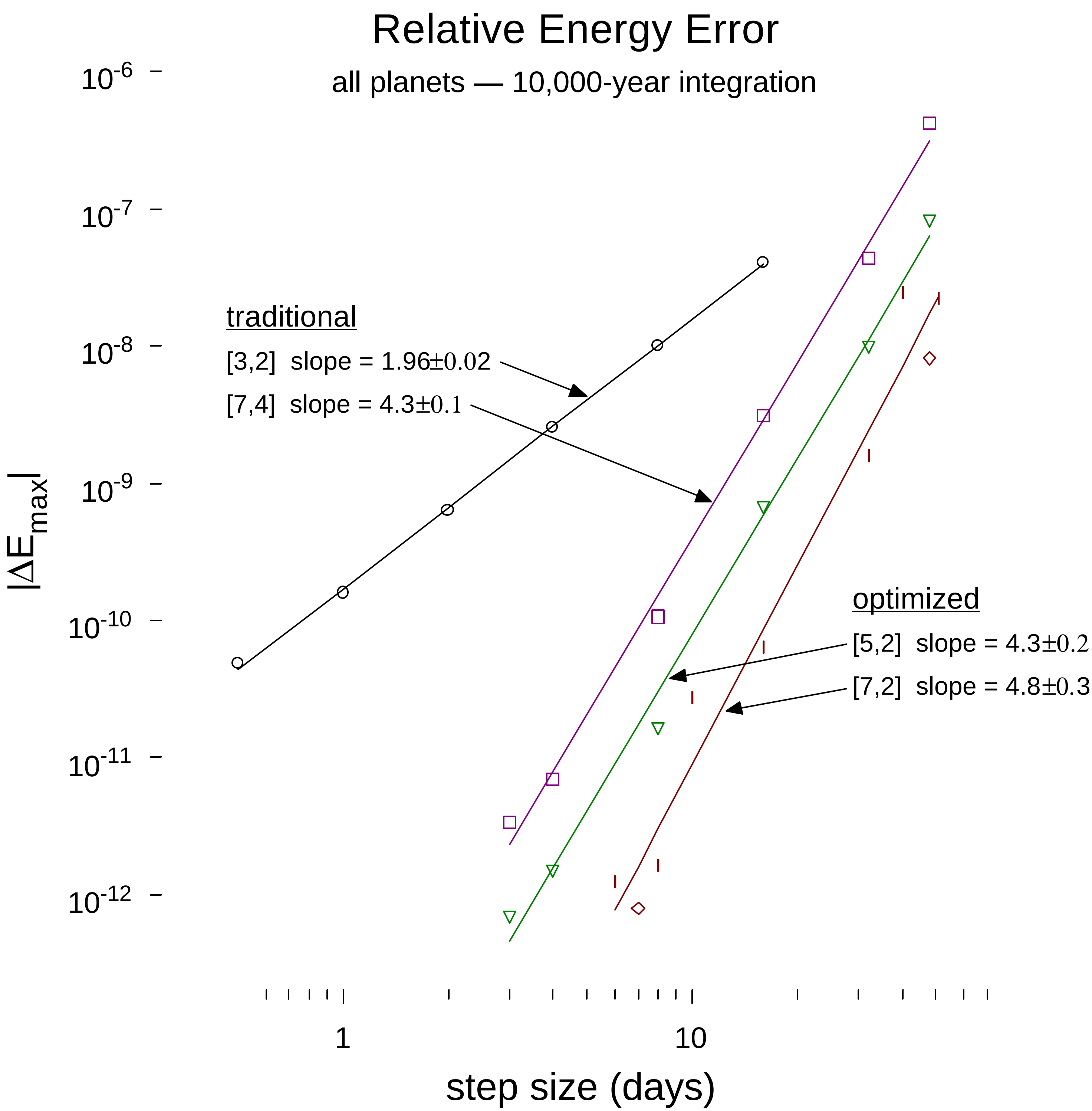
Preliminary Numerical Results (continued)

- Results:
  - For traditional [3,2] and [7,4] methods, max energy error goes as τ^2 and τ^4, as expected
  - For optimized [5,2] and [7,2] methods, max energy error goes as τ^4 and τ^6
  - The optimized methods cost significantly less in CPU time than the traditional methods
    - even [7,2] is less costly than [3,2] at higher accuracies!

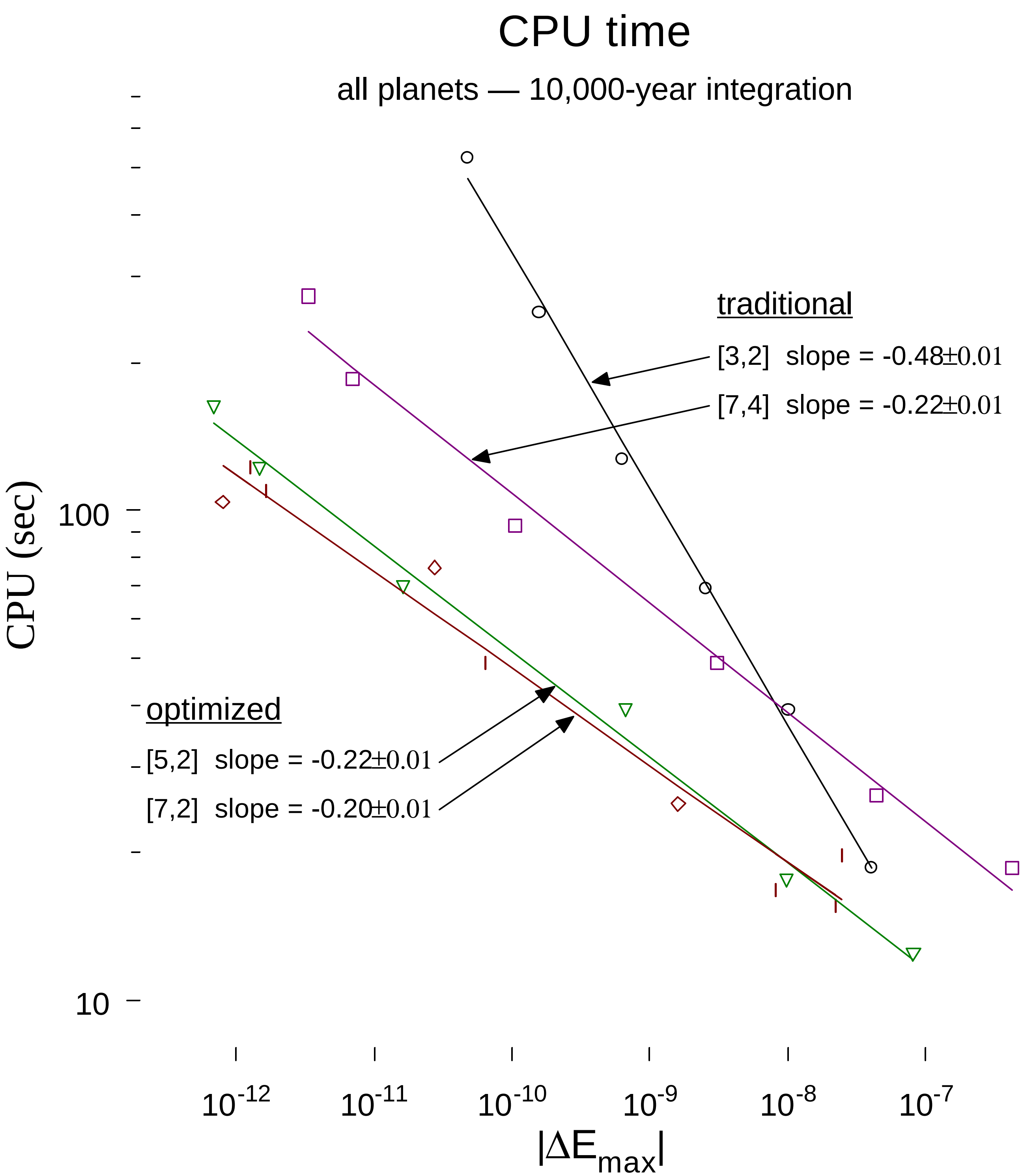


Relative Energy Error
terrestrial planets — 10,000-year integration
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
$|\Delta E_{max}|$
traditional
[3,2] slope = 2.02±0.02
[7,4] slope = 3.9±0.2
optimized
[5,2] slope = 4.5±0.2
[7,2] slope = 6.4±0.3
1
10
step size (days)


CPU time
terrestrial planets — 10,000-year integration
CPU (sec)
100
10
traditional
[3,2] slope = -0.454±0.009
[7,4] slope = -0.23±0.01
optimized
[5,2] slope = -0.183±0.009
[7,2] slope = -0.135±0.007
10^{-12}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
$|\Delta E_{max}|$



Relative Energy Error
all planets — 10,000-year integration
$|\Delta E_{max}|$
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
traditional
[3,2] slope = 1.96±0.02
[7,4] slope = 4.3±0.1
optimized
[5,2] slope = 4.3±0.2
[7,2] slope = 4.8±0.3
1
10
step size (days)



CPU time
all planets — 10,000-year integration
traditional
[3,2] slope = -0.48±0.01
[7,4] slope = -0.22±0.01
optimized
[5,2] slope = -0.22±0.01
[7,2] slope = -0.20±0.01
CPU (sec)
100
10
10-12
10-11
10-10
10-9
10-8
10-7
|ΔEmax|

Preliminary Conclusions

- This is fun!
- The approach outlined in this talk yields optimized low-order (in time step) symplectic methods that can perform as well as higher-order methods, but at significantly less cost.

To Do

- Teach SYMPLECTIC new tricks
  - better intermediate expression simplification
    - expressions occupy tens of megabytes
    - requires ~100 MB and more of "running room" (i.e., RAM)
    - ➡ handle complicated nested sqrts (easy)
    - ➡ represent error expressions in a commutator notation (hard!)
    - ➡ Take advantage of BCH formula
  - eliminate selected ε^2 subterms
- Complete the exploration of the
  [exp terms, step order]
  space out to current software (Maple) and hardware (memory, speed) limits
- Complete the numerical comparisons of each of the optimized methods
- 2nd AJ paper